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14. ABSTRACT

The goal of this proposal is to model the stability of quantum states of matter derived from topological insulators against two types of corrections: strong inter-particle interactions and heating. I will examine interacting atoms in square optical lattices with spin orbit coupling, and more generally, gauge fields, as a route to building Hubbard models hosting fractional topological insulators. I will analyze these models by combining numerical exact diagonalization on small lattice clusters with an analytic variational theory. I also propose to study a new model of

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Final Report: Modeling the Stability of Topological Matter in Optical Lattices

ABSTRACT

The goal of this proposal is to model the stability of quantum states of matter derived from topological insulators against two types of corrections: strong inter-particle interactions and heating. I will examine interacting atoms in square optical lattices with spin orbit coupling, and more generally, gauge fields, as a route to building Hubbard models hosting fractional topological insulators. I will analyze these models by combining numerical exact diagonalization on small lattice clusters with an analytic variational theory. I also propose to study a new model of finite temperature topological superconductors of dipoles placed in an optical lattice. I will construct and analyze a model using a combination of mean field theory and quantum Monte Carlo. The proposed work will foster new directions in experiments with optical lattices containing cold atomic gases. These new states of matter should exhibit new particles as excitations. Analyses of the stability of these new topological phases will thus play a crucial role in advancing fundamentally new directions in physics.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

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TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received   Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Conferences:

APS March Meeting 2013, Baltimore, MD
Authors: F. Lin, V. W. Scarola
Title: Enhancing the thermal stability of entanglement between Majorana fermions with dipoles in optical lattices

APS March Meeting 2013, Baltimore, MD
Authors: Yinyin Qian, Ming Gong, Vito Scarola, Chuanwei Zhang
Title: Phase-modulated superfluids of bosons in spin-orbit coupled optical lattice

APS March Meeting 2013, Baltimore, MD
Authors: F. Lin, V. W. Scarola
Title: Flat-band engineering of interactions in spin-orbit coupled optical lattices

Other Presentations:

ARO Atomtronics Review Meeting, College Park, MD
Authors: F. Lin, V. W. Scarola
Title: Enhancing the thermal stability of entanglement between Majorana fermions with dipoles in optical lattices

Oakridge National Lab, Oakridge, TN
Presenter: V.W. Scarola
Title: Strongly Correlated Atoms in Optical Lattices

Boston University, Boston MD
Presenter: V.W. Scarola
Title: Strongly Correlated Atoms in Optical Lattices

Number of Presentations: 0.00

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Received   Paper

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Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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(d) Manuscripts

Received	Paper

05/16/2013 1.00 Yinyin Qian, Ming Gong, V. W. Scarola, Chuanwei Zhang. Dzyaloshinskii-Moriya Interaction and Spiral
Order in Spin-orbit Coupled Optical Lattices,
ArXiv e-prints (05 2012)

05/16/2013 2.00 Fei Lin, Vito W. Scarola. Enhancing the thermal stability of entanglement between Majorana fermions with
dipoles in optical lattices,
ArXiv e-prints (09 2012)

TOTAL: **2**

Number of Manuscripts:

Books

Received	Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Dr. Fei Lin	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Vito Scarola	0.08	
FTE Equivalent:	**0.08**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

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This section only applies to graduating undergraduates supported by this agreement in this reporting period

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Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

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Names of Personnel receiving masters degrees

NAME
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Names of personnel receiving PHDs

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Total Number:

Names of other research staff

NAME		PERCENT SUPPORTED
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Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Please see the attached pdf.

Technology Transfer

Final Report: Modeling the Stability of Topological Matter in Optical Lattices
PI: Asst. Prof. Vito Scarola, Virginia Tech Dept. of Physics

Technical Point of Contact: Paul Baker, Atomic and Molecular Physics
Short Term Innovative Research (STIR) Program

Project Abstract

The goal of this proposal is to model the stability of quantum states of matter derived from topological insulators against two types of corrections: strong inter-particle interactions and heating. I will examine interacting atoms in square optical lattices with spin orbit coupling, and more generally, gauge fields, as a route to building Hubbard models hosting fractional topological insulators. I will analyze these models by combining numerical exact diagonalization on small lattice clusters with an analytic variational theory. I also propose to study a new model of finite temperature topological superconductors of dipoles placed in an optical lattice. I will construct and analyze a model using a combination of mean field theory and quantum Monte Carlo. The proposed work will foster new directions in experiments with optical lattices containing cold atomic gases. These new states of matter should exhibit new particles as excitations. Analyses of the stability of these new topological phases will thus play a crucial role in advancing fundamentally new directions in physics.

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(2) Statement of The Problem Studied

The goal of the STIR proposal was to study the stability of quantum states of matter derived from topological insulators against two types of corrections: strong inter-particle interactions and heating. These parameters can be tuned and controlled in optical lattices while leaving out other influences by construction.

We studied strong spin orbit coupled problems to set the stage for further work on topological states of matter. Topological states of matter are derived from strong spin orbit interaction in the context of topological insulators and topological superconductors. In section 3A I discuss work that studies the thermal stability of topological superconductors, in section 3B I discuss work that builds a formalism to study the competition between strong interaction and strong spin orbit coupling. In section 3C I discuss results on the search for topological states in the presence of strong spin orbit coupling and strong interactions between fermions in an optical lattice. And finally, in section 3D, I discuss results that studies strong interaction and strong spin orbit coupling between bosons in an optical lattice.

The work started here can be used to study topological states of matter in more realistic settings. Comparison with and predictions for experiments are now a possibility. Furthermore the methods and techniques constructed here can be generalized to apply to other systems: quantum wire arrays containing topological superconductors, quantum Hall effects, fractional Chern insulator lattice models, and fractional topological insulators.

(3) Summary

3A: Enhancing the thermal stability of entanglement between Majorana fermions with dipoles in optical lattices
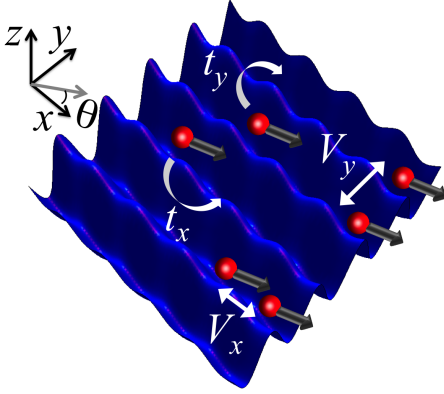

Figure 1: Schematic of dipolar fermions (spheres) in a 2D optical lattice. Dipolar moments (arrows on each sphere) align along an applied field, at an angle θ with the x-axis. The optical lattice depth is large along the y direction.

The wide variety of optical lattice geometries offer unprecedented tunability in manipulating quantum degenerate gases into complex quantum states. Recent developments in the cooling of molecules and magnetic atoms imply that anisotropy in dipolar interactions will soon provide further opportunity to explore some of the most elusive yet compelling quantum states, entangled Majorana fermions (MFs). Fig. 1 shows a figure of a lattice model we studied.

Certain models demonstrate particle-like excitations that behave as MFs thanks to peculiar non-local symmetries. MFs are their own antiparticles. They entangle with each other over large distances through string operator correlations, signaling underlying topological order with fascinating properties that have motivated proposals for topologically protected qubits. The crossing of string operators is responsible for unusual anyonic braid statistics. And string operators connecting these excitations also underly theories of quantum state teleportation.

The zero-temperature properties of models hosting topological order set the stage for work connected to experiments. Kitaev's two-dimensional (2D) Toric Code Hamiltonian motivated early proposals in optical lattices containing ultracold atoms, polar molecules, and atoms in Rydberg states. But the 1D Kitaev chain model is one of the simplest models supporting free MF excitations. Anticipation of non-local MF properties in 1D led to experimental proposals in both optical lattices and solids, and recent experiments in quantum wires. But prospects for observing interesting effects due to non-local correlation of MF pairs over long times and distances hinge on the stability of string operators.

String operators in important lattice models are unstable at non-zero temperatures, e.g., string operators in the 2D Toric Code model vanish at long times and distances because of thermal excitations. Recent work also argues that MFs in lattice models of topological p-wave superconductors are sensitive to thermal fluctuations.

We addressed the issue of thermal stability by showing that anisotropic interactions between dipolar fermions in optical lattices can be used to significantly enhance thermal stability [1]. We constructed a model of oriented dipolar fermions in a square optical lattice. Our model reduces to an interacting Kitaev chain model of fermions hoping with an energy t along chains. We found that domains established by strong interactions

exhibit enhanced correlation between Majorana fermions over large distances and long times even at finite temperatures, suitable for stable redundancy encoding of quantum information. Our approach can be generalized to a variety of configurations and other systems, such as quantum wire arrays.

Fig. 2 shows one of our key results. The expectation value of the string operators, P_j, act as order parameters. Unique values, $\langle P_j \rangle = \pm 1$, can be used to define each sector and therefore indicate stability in the string operators of MFs. But $\langle P \rangle = 0$ indicates that thermal excitations destroy any distinction between sectors. We compute $\langle P_j \rangle$ explicitly on a model describing strongly interacting Kitaev wires to show indications of spontaneous breaking of these discrete symmetries for even at non-zero temperatures. To detect such a symmetry breaking we perturb the above spinless fermion model with a weak global field of strength h. The global field imposes a splitting between the otherwise degenerate states. Our results clearly show the thermal robustness of Majorana fermions in our model.

We considered an effective model of oriented dipolar fermions in a 2D lattice that allows hopping along directions
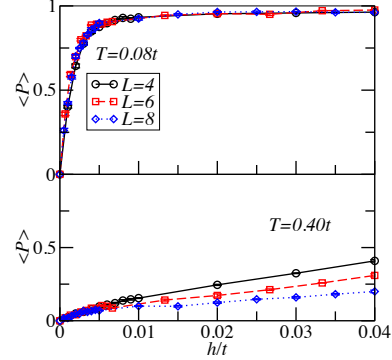

Figure 2: The thermal expectation value of string operators from quantum Monte Carlo as a function of an applied global field for several system sizes, L. The top (bottom) panel shows data for a characteristic low (high) temperature.

where the dipoles attract but suppresses hopping along directions where dipoles repel. We also performed unbiased QMC to directly check that string operators defining non-local MF states remain robust to thermal fluctuations. This class of models also applies to Coulomb-coupling in MF models of quantum wire arrays or quasi-1D tubes containing topological superconductors.

Strongly correlated systems can often be understood using wavefunctions constructed from Jastrow factors that lower interaction energies by separating particles. A useful interpretation of Jastrow factors based on vortices (wavefunction zeroes) views a Jastrow factor as tool to introduce vortices into an otherwise weakly correlated system. Careful tuning of the location of each vortex optimizes energetics of individual problems. This procedure has proven to be quantitatively useful in combination with stochastic methods in quantum chemistry and other fields.

Vortex insertion with Jastrow factors has been the tool of choice in highly successful theories of the quantum Hall regime. In the quantum Hall regime the kinetic energy is quenched leaving the interaction to operate in a flat band. The Hamiltonian has no small parameters and thus defines a challenging many-body problem. In this regime the success of quantum Hall ansatz wavefunctions shows that vortex attachment to each particle helps screen the otherwise strong inter-particle repulsion by tuning the size of correlation holes.

Flat band models have recently been shown to describe a wealth of other quantum many-body systems. These include graphene-based nanostructures, fast rotating atomic gases, kagome lattices, fractional Chern insulators, and strongly spin-orbit coupled systems, to name a few. The success of the quantum Hall wavefunctions in capturing the essential physics of the Coulomb interaction within a flat Landau level suggests that vortex attachment to particles might be a quantitatively useful ansatz in solving these other flat-band problems as well. Vortex attachment may also be used to study fractional topological insulators.

We constructed a formalism that uses a basis-independent representation of Jastrow factors to attach vortices in the matrix product setting [2]. We then tested this formalism on a few examples. We showed that the formalism can be used to directly write the single component Laughlin states in terms of matrix products. We also used the formalism to solve a flat-band problem that does *not* have a polynomial basis representation: two-dimensional helical fermions in the presence of strong Rashba spin-orbit coupling. This problem is of direct relevance to ongoing experiments with ultracold atomic gases. We found that interactions in a flat spin-orbit band favor the formation of a central vortex in analogy to what has been found in studies of rotating quantum gases and quantum dots. The formalism allows straightforward validation of Jastrow-correlated ansatz states in small system sizes and sets the stage for optimization of these wavefunctions with efficient matrix product algorithms. We are currently preparing a manuscript for submission [2].
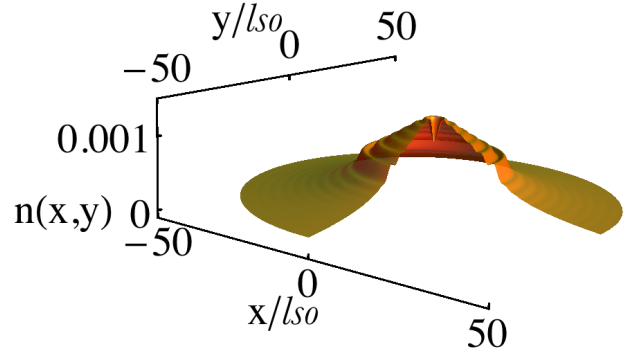

Figure 3: The density of a "vortex core" ansatz state of helical fermions in the presence of Rashba spin orbit coupling plotted as a function of x and y in units of the spin-orbit length l_{SO}.

The primary result was a comparison of ansatz wavefunctions and results from exact diagonalization. The overlaps between the ansatz and exact states were better than 98%. Fig. 3 shows the density in the plane for the successful state. The vortex in the system center helped minimize the interaction energy.

Emergent excitations can have properties that are not restricted by common symmetries. One of the best known examples is in the fractional quantum Hall regime where many-body effects in a quantum flat-band lead to excitations with topological properties. These topological excitations can have, for example, fractional charge.
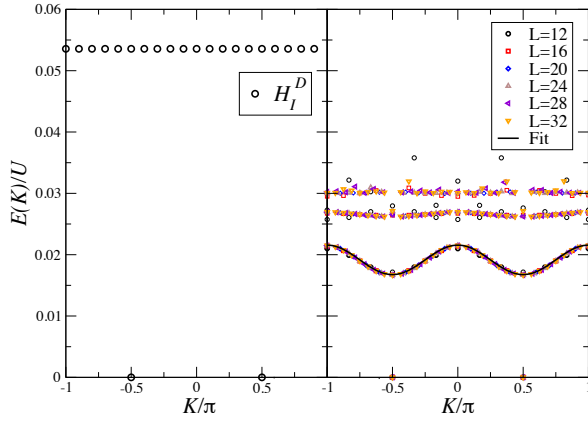

Figure 4: Left: Plot of the many-body energy of a diagonal nearest neighbor interaction as a function of wavevector. The ground state is a Wigner crystal and the excitations are classical. Right: The same but for a flat spin-orbit band. The ground state is still a Wigner crystal but the excitations are show an emergent dispersion due to quantum effects.

Recent cold atom experiments have made an important breakthrough in realizing spin-orbit couplings, which opened a door to realizing flat quantum bands. We find that strong interactions in this flat band leads to intriguing excitations with fractional charge.

We are currently preparing our manuscript to report results that explores these issues in optical lattices [3]. We constructed a tight-binding Hamiltonian for a spin-orbit coupled Fermionic optical lattice system, and perform flat-band projection of on-site interactions to generate longer-range interactions between flat-band particles. We solved the resultant projected interacting Hamiltonian with exact diagonalization at some parameter regime, and obtained spinor Wigner crystal ground state with an emergent kinetic bands above the ground state. We deduce an effective extended Hubbard model with modulated next nearest neighbor hoppings to describe the emergent kinetic bands. Emergent dispersive bands are shown in Fig. 4. The effective model then leads to charge fractionalization of the elementary Bosonic excitations, revealed in the conventional bosonization approach.

In this work [4] we showed that the recent experimental realization of spin-orbit coupling in ultracold atomic gases can be used to study different types of spiral order and resulting multiferroic effects. Spin-orbit coupling in optical lattices can give rise to the Dzyaloshinskii-Moriya spin interaction which is essential for spin spiral order. We derived an effective spin model in the deep Mott insulator region at half filling, and demonstrate that the Dzyaloshinskii-Moriya interaction in optical lattices can be made extremely strong with realistic experimental parameters. The rich phase diagrams of the effective spin model for fermion and bosons are obtained via classical Monte Carlo simulations.

The interplay between ferro-electric and ferromagnetic order in complex multiferroic materials presents a set of compelling fundamental condensed matter physics problems with potential multifunctional device applications. Ferroelectric and ferromagnetic order compete and normally cannot exist simultaneously in conventional materials. Coexistence of these orders often relies on strong correlation. In some strongly correlated systems, such as the perovskite transition metal oxides, these two phenomena can occur simultaneously. Construction and design of high-T_c magnetic ferroelectrics is still an open and active area of research. These and other complex
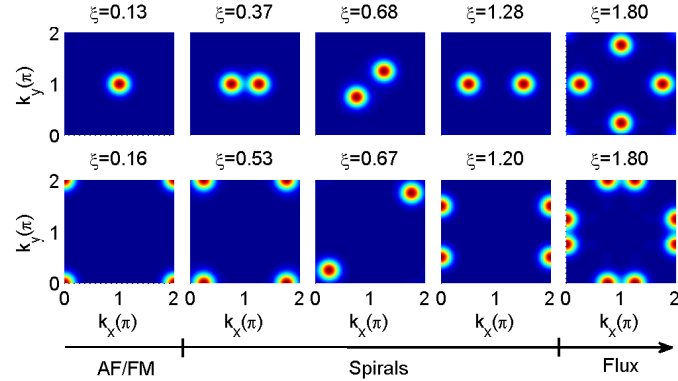

Figure 5: Spin structure factors for different quantum phases. The upper panels show the results for fermions, while the lower panels show the results for bosons.

solids incorporate different types of interactions, including electron-electron interactions, electron-phonon interactions, spin-orbit couplings, lattice defects, and disorder, making the determination of multiferroic mechanisms a remarkable challenge for most materials. Due to the inherent complexity of the different interactions involved, the underlying mechanism for the emergence of multiferroic behavior is not fully clear. An unbiased and direct method to explore multiferroic behavior (e.g., dynamics, critical exponents, the impact of controlled disorder, etc.) in an ideal setting is thus highly appealing.

We showed that the power of optical lattice systems to emulate magnetism can be combined with recent experimental developments realizing spin-orbit coupling to emulate multiferroic behavior. Recently, spin-orbit coupled optical lattices have been shown to possess flat energy band, and important experimental progress has been made for observing the single particle band dispersion (including the flat band) in spin-orbit coupled optical lattices. The main findings of this work are the following: (I) We derive the effective Hamiltonian for spin-1/2 fermions and bosons in optical lattices in the large interaction limit. We show that spin-orbit coupling leads to an effective in-plane Dzyaloshinskii-Moriya term, an essential ingredient in models of spiral order and multiferroic effects in general. We estimate that the DM term is of the same order as the Heisenberg coupling

constant, J. (II) We study the phase diagram of the effective spin model using classical Monte Carlo. We find that competing types of spiral order depend strongly on the spin-orbit coupling strength and effective Zeeman field. Fig. 5 shows examples of the spin structure factor used to identify phase transitions. (III) We find that the critical temperature for the spiral order can be made rather high. Thus, if magnetic quantum phase transitions can be emulated in optical lattices, then spiral order and multiferroics can also be realized in the same setup with the inclusion of spin-orbit coupling.

(4) Bibliography

[1] Fei Lin and V.W. Scarola, Enhancing the thermal stability of entanglement between Majorana fermions with dipoles in optical lattices, Preprint: arXiv:1210.0799 (2013).

[2] V.W. Scarola, Vortex attachment via matrix products: application to flat spin-orbit bands, Manuscript in preparation (2013).

[3] Fei Lin and V.W. Scarola, Flat-band engineering of interactions in spin-orbit coupled 1D optical lattices, Manuscript in preparation (2013).

[4] Ming Gong, Yinyin Qian, V. W. Scarola, and Chuanwei Zhang, Dzyaloshinskii-Moriya Interaction and Spiral Order in Spin-orbit Coupled Optical Lattices, Preprint: arXiv:1205.6211 (2012).